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PARTITIONING OPTICAL PROPERTIES INTO ORGANIC AND INORGANIC COMPONENTS FROM OCEAN COLOR IMAGERY

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ABSTRACT

Current ocean color satellite algorithms generally partition the total absorption coefficient into two components, one due to phytoplankton and one due to the combined effect of detritus and colored dissolved organic matter (CDOM, or gelbstoff). Detritus and CDOM exhibit similar spectral shapes so they are typically modeled together. The separation of the particulate phase into organic and inorganic components through remote sensing has only recently been addressed. We present algorithms to estimate the concentrations of total suspended solids (TSS), particulate organic matter (POM), and particulate inorganic matter (PIM) from SeaWiFS imagery. Furthermore, we partition the combined CDOM/detrital absorption coefficient into separate components, and using a previously published algorithm, we partition the scattering coefficient (b) into organic (b_o) and inorganic (b_i) components.

Using *in situ* ac9 data (unfiltered and filtered through a 0.2 micron filter) collected in Mississippi Bight, we developed an empirical algorithm to calculate CDOM absorption separately, through a regression relationship with the total absorption coefficient. We then estimate particulate and detrital absorption through subtraction. We use the particulate absorption at 412 and 443 nm (derived from ac9 and filter pad data) to estimate PIM and POM, and subsequently TSS as the sum. During our study periods, we observed a strong relationship between PIM and TSS; PIM represented 76% of TSS in both offshore waters and in turbid coastal waters with TSS values as high as 60 mg/l ($R^2 = 0.986$). We apply these algorithms to SeaWiFS data and present examples of the new satellite ocean color products.

INTRODUCTION

The optical separation of organic and inorganic particulate matter has been problematic. Spectrally, the absorption coefficients of both CDOM and detritus exhibit an exponential decay with increasing wavelength in the visible, so current ocean color algorithms model these together as one combined term (a_{dg}). With the development of the ac9 instrument and the capability to attach a 0.2 μm pre-filter to the intake of the instrument, routine measurements of CDOM absorption are now common, and more extensive data sets of both dissolved and particulate absorption are now becoming available, particularly when the instruments are used in flow-through mode over large areas. In addition, filter pad absorption techniques also allow separation of the total absorption coefficient into components due to CDOM, phytoplankton, and detritus. Nevertheless, satellite ocean color algorithms fail to distinguish between CDOM and detrital absorption (Garver and Siegel, 1997).

The concentration of total suspended solids, and its partitioning into organic and inorganic components is also of interest from both remote sensing and modeling aspects. The concentration and space/time distribution of the inorganic component (sediments, both river-borne and resuspended) can be used to trace river plumes and fronts, and can indicate regions of increased turbulence due to wave action and storm events. The distribution of the organic component does not necessarily mirror the distribution of the inorganic component, as they are influenced by different processes (physical vs. biological controls). So, it would be advantageous to develop algorithms to remotely estimate both the concentrations and the optical characteristics (absorption, scattering coefficients) of the organic and inorganic constituents of the water.

We present simple empirical algorithms to estimate the concentrations of PIM, POM, TSS, and acDOM, from SeaWiFS imagery. We recognize that empirical algorithms inherently suffer from a regional dependence and may only be valid for the regions and time periods used in their development. We are evaluating the algorithms over broader areas and, in the future, we will compare the results with *in situ* measurements and a more analytical approach based on refractive indices, particle size distributions, and Mie theory recently presented by Twardowski et al. (2001).

METHODS

During 2001 and 2002, we collected a suite of optical measurements in Mississippi Bight, in both clear offshore waters and turbid coastal waters. Station locations during 19-25 May 2002 are indicated in Figure 1, for the two research vessels involved, the R/V Ocean Color and the R/V Pelican. The Pelican mapped the outflow plume from Mobile Bay while the Ocean Color examined spatial variability of optical properties in Mobile Bay and Mississippi Sound (shoreward of the barrier islands).

On both vessels, ac9 instruments were deployed both with and without 0.2 μm filters attached to the intake tubes, to separate the total absorption into dissolved and particulate components. Ac9 data were temperature and scatter corrected. On the Pelican, vertical casts as well as flow-through data were collected, while on the Ocean Color, only vertical station casts were collected. In addition, whole water samples were

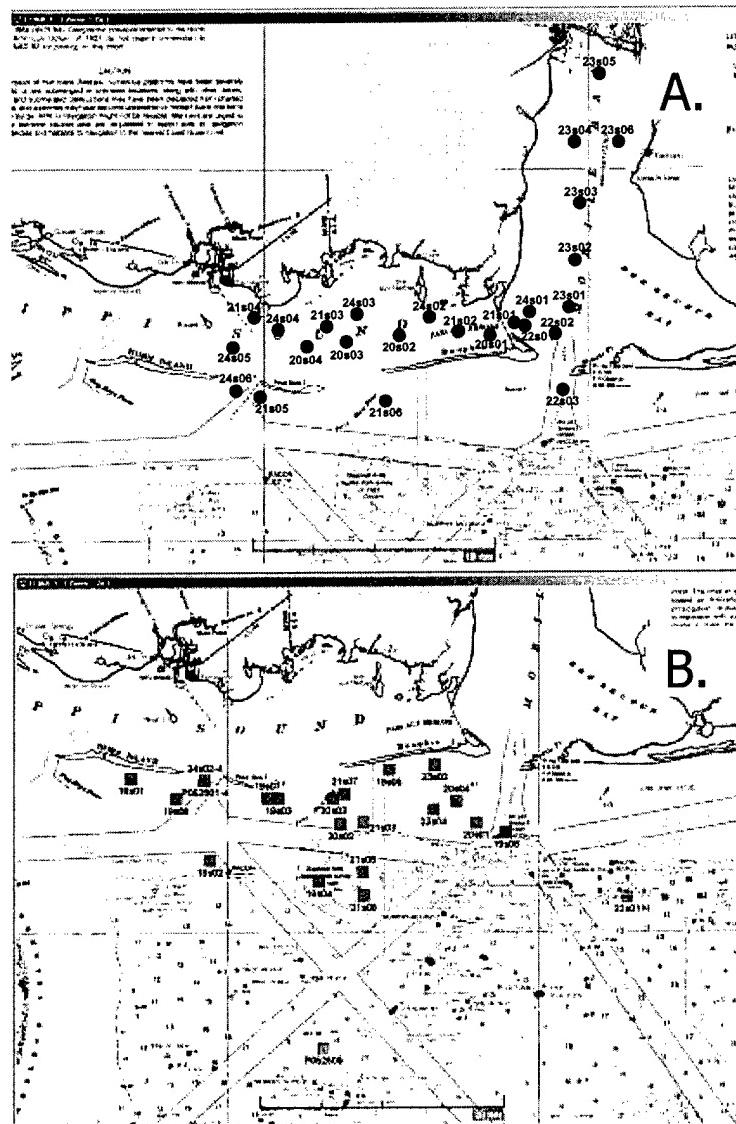


Figure 1. Station locations, May 2002. Mississippi Sound and Mobile Bay
A. R/V Ocean Color. B. R/V Pelican.

collected on both ships and filter pad absorption analyses were performed (a_p , a_{CDOM} , a_ϕ , a_d) using a fiber optic ASD VNIR field spectroradiometer. Chlorophyll was measured fluorometrically and filtered samples were collected and frozen in liquid nitrogen for HPLC analysis. TSS, PIM, and POM were determined gravimetrically. Prior to the cruise, 47 mm GF/F filters were rinsed three times with Milli-Q water, dried for two hours at 103° C, ashed for 15 minutes at 550° C, weighed on an analytical scale, and stored for analysis in small, labeled plastic petri dishes. During the experiment, whole water samples were subsequently filtered through the prepared filters, rinsed thoroughly, dried, and weighed to determine TSS in mg/l. The volume filtered varied between samples (depending on whether the sample was collected in clear offshore waters or sediment-laden nearshore waters), but in each case filtration continued until the filter was

nearly clogged, to ensure maximal loads for the gravimetric analysis. The filters were then ashed and re-weighed to determine PIM (and POM through subtraction).

RESULTS

To separate the absorption coefficient into dissolved and particulate components from remote sensing imagery, we first developed a simple empirical relationship between the total absorption coefficient at 412 nm, with water absorption removed, $a_{t-w}(412)$, and the absorption coefficient due to CDOM at 412 nm, $a_{CDOM}(412)$, using the *in situ* filtered and unfiltered ac9 data sets from both years (Figure 2A). A second-order polynomial fit to the data (with a forced intercept of 0) yielded:

$$a_{CDOM}(412) = 0.7696 a_{t-w}(412) - 0.08858 a_{t-w}(412)^2 \quad (1)$$

with an R^2 value of 0.80. Note the large spread in the data indicating substantial variability. To derive estimates of a_{CDOM} at other wavelengths, we plotted a_{CDOM} at each ac9 wavelength against $a_{CDOM}(412)$; slopes were calculated from least-squares linear regression (Figure 2B). This is similar to the approach of Gould et al. (1999) to calculate the shape of spectral scattering. Next, the regression slopes, M, were plotted against wavelength (Figure 2C), and a non-linear least-squares analysis was performed to fit the model:

$$M = C1 e^{(-C2(\lambda-400))} \quad (2)$$

Thus,

$$a_{CDOM}(\lambda) = a_{CDOM}(412) * [C1 e^{(-C2(\lambda-400))} / C1 e^{(-C2(412-400))}] \quad (3)$$

With the derived values of C1 and C2 from Figure 2C (1.20809 and 0.0167, respectively), this equation reduces to:

$$a_{CDOM}(\lambda) = a_{CDOM}(412) * 1.22189 e^{(-0.0167(\lambda-400))} \quad (4)$$

Because we can estimate $a_{t-w}(412)$ from SeaWiFS imagery, (Carder et al., 1999), we can subsequently derive remote sensing estimates of spectral $a_{CDOM}(\lambda)$ from the equations above. Particulate absorption is calculated by difference:

$$a_p(\lambda) = a_{t-w}(\lambda) - a_{CDOM}(\lambda) \quad (5)$$

Using previously developed relationships for phytoplankton absorption, a_ϕ (Carder et al., 1999), detrital absorption is also calculated by difference:

$$a_d(\lambda) = a_p(\lambda) - a_\phi(\lambda) \quad (6)$$

Figure 3 shows examples of $a_{CDOM}(412)$ and $a_p(412)$ derived from SeaWiFS imagery collected on 20 May, 2002, during our Mobile Bay experiment.

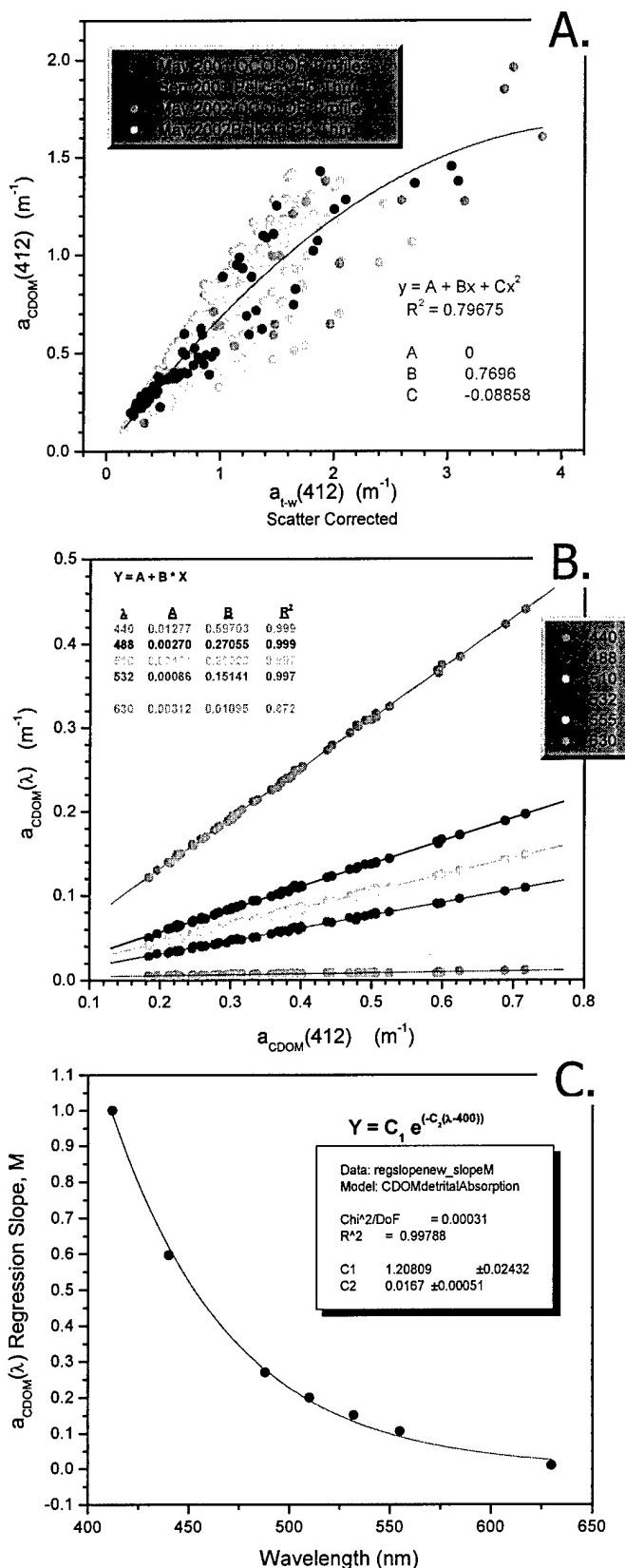


Figure 2. A. $a_{CDOM}(412)$ vs $a_{t-w}(412)$, from filtered and unfiltered ac9 data. B. $a_{CDOM}(\lambda)$ vs. $a_{CDOM}(412)$. C. Regression slopes (from equations in B) vs. wavelength.

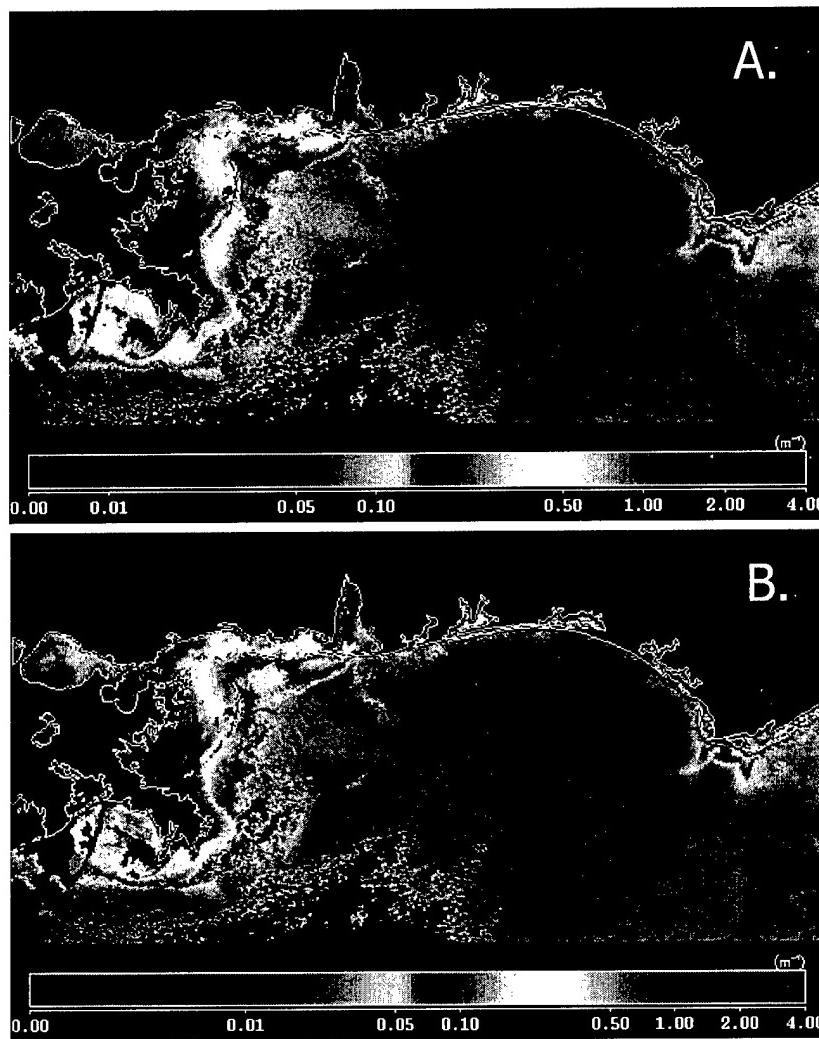


Figure 3. SeaWiFS imagery, May 20, 2002. A. $a_{CDOM}(412)$. B. $a_p(412)$. Black pixels are clouds

During both years, we observed a strong relationship between *in situ* measurements of the scattering coefficient at 555 nm, $b(555)$, and TSS (Figure 4A). This is not unexpected, as the suspended particulate matter is the source of the optical scattering. However, we also observed a very strong and consistent relationship between PIM and TSS in this region during May 2002, with samples spanning the entire range from nearshore to offshore conditions (Figure 4B). The regression slope was 0.76, indicating that the inorganic contribution to the total particulate load remained constant at 76%, with an R^2 value of 0.986. This is somewhat surprising and indicated low spatial variability of the inorganic material, relative to the total. However, the entire area is dominated by river discharge from the Mobile and Pascagoula Rivers, and measurements were collected over a relatively short period (1 week). Greater variability was observed in the nearshore samples relative to offshore (red vs. blue points, respectively, in Figure 4B).

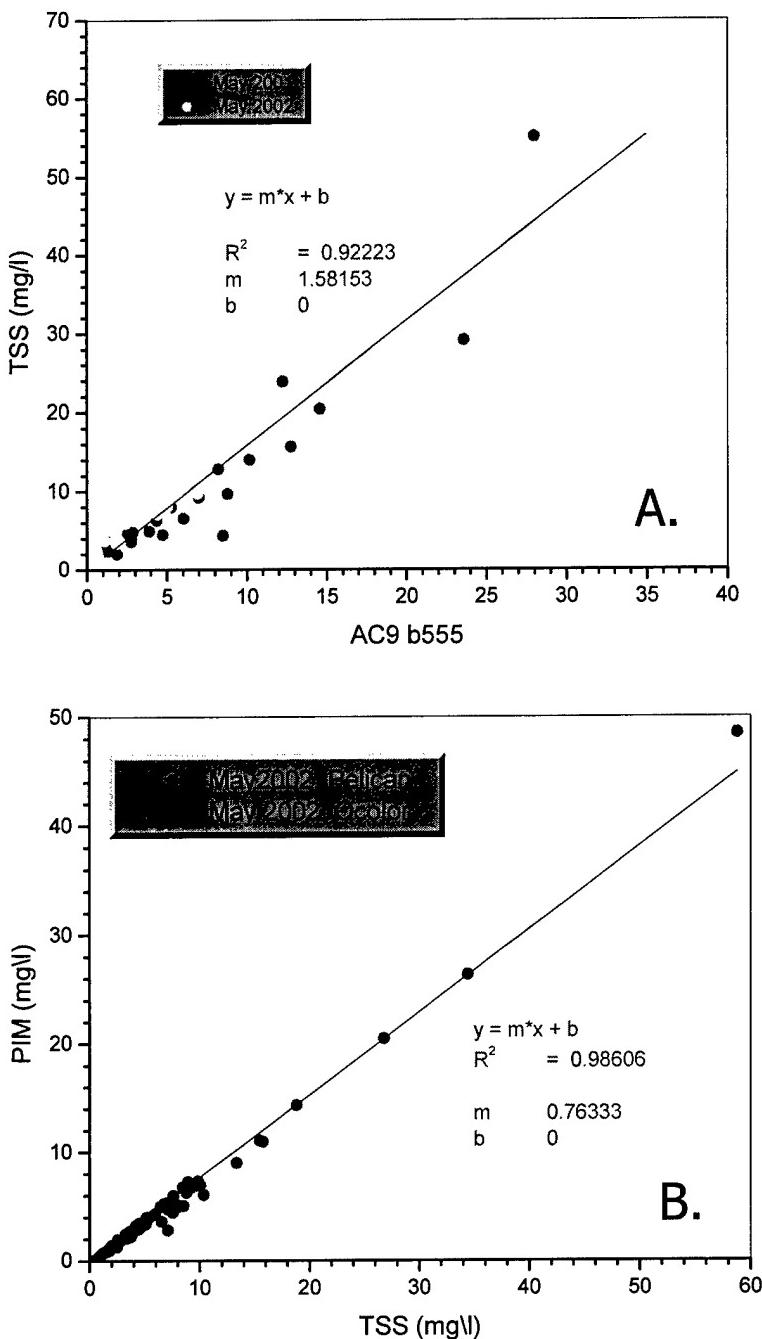


Figure 4. A. TSS vs. b(555). B. PIM vs. TSS.

To estimate POM, we regressed measured values of POM against particulate absorption at 443 nm, $a_p(443)$, derived from the filter pad analyses at the stations. The rationale for this derives from an expected relationship between organic matter concentration and absorption due to chlorophyll at 443 nm, under the assumption that the distributions of organic matter and chlorophyll-containing particles co-vary (as in the calculation for scattering due to organic matter, see below). Undoubtedly, this may not

always be the case. Similarly, to estimate PIM, we regressed measured values of PIM against the filter pad measurements of particulate absorption at 412 nm, $a_p(412)$. These relationships and least-squares regressions are shown in Figures 5A and 5B. Note that at higher particulate absorption values, POM tends to level off while PIM continues to increase and level off more slowly, suggesting that the inorganic component will become more dominant in coastal waters. TSS is calculated as the sum of PIM and POM. Figures 6A, B, and C show examples of POM, PIM, and TSS derived from SeaWiFS imagery collected on 20 May, 2002, during our Mobile Bay experiment.

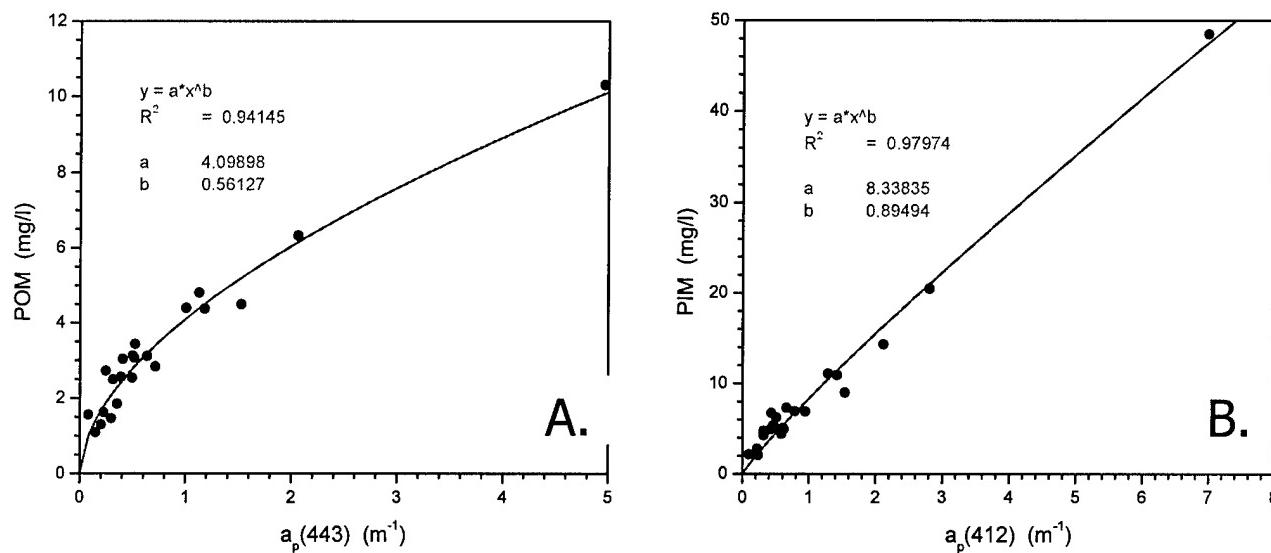


Figure 5. A. POM vs. $a_p(443)$. B. PIM vs. $a_p(412)$.

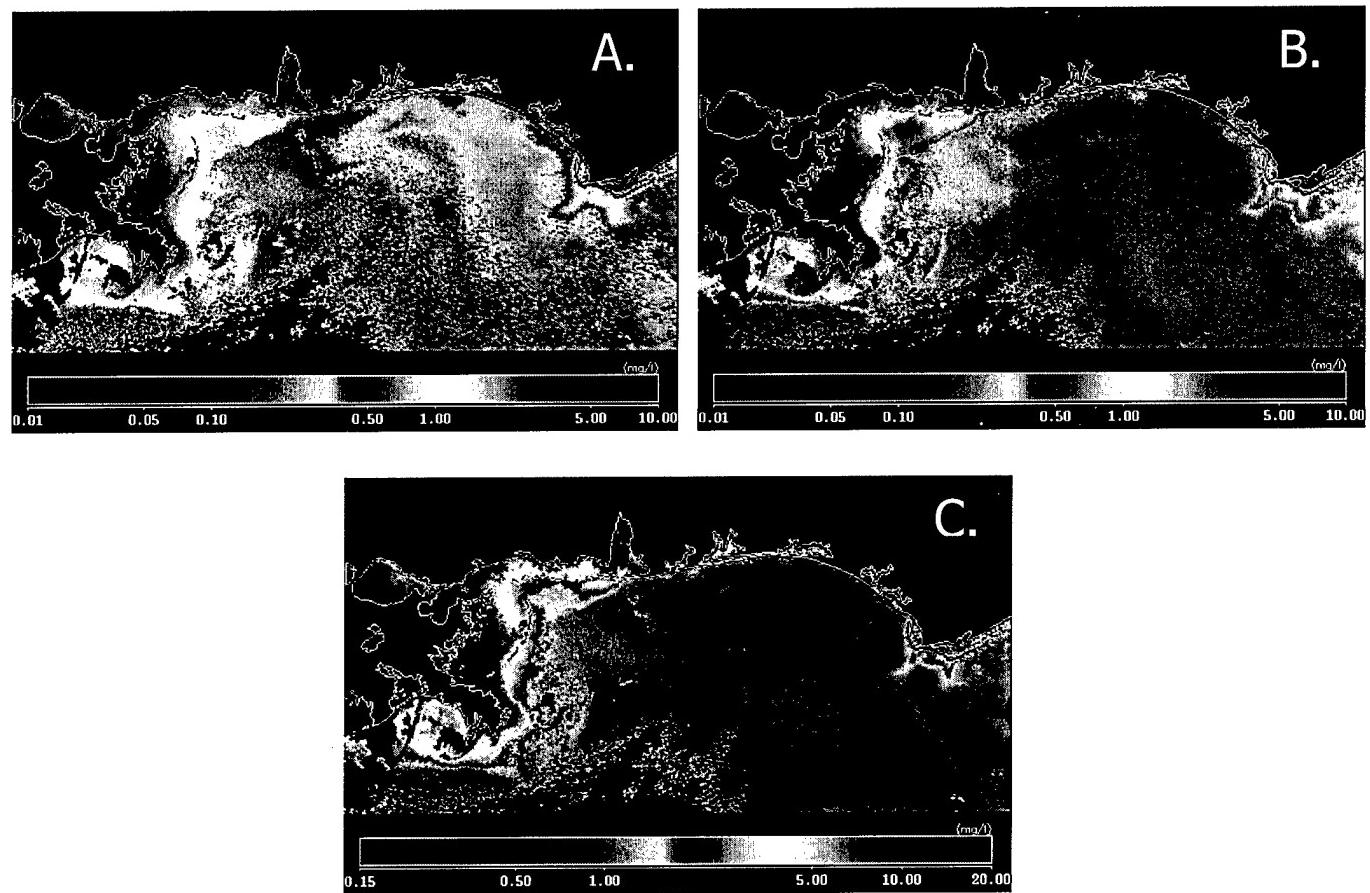
Finally, we partitioned the total scattering coefficient into organic, b_o , and inorganic, b_i , components, using the relationships developed in Loisel and Morel (1998). They related the beam attenuation coefficient at 660 nm to the chlorophyll concentration and suggested that at that wavelength, approximately 97% of the particle attenuation coefficient was due to particle scattering. Thus, using a $1/\lambda$ spectral dependence:

$$b_o(555) = (0.189 \text{ CHL}^{0.751}) * 0.97 * 660/555 \quad (7)$$

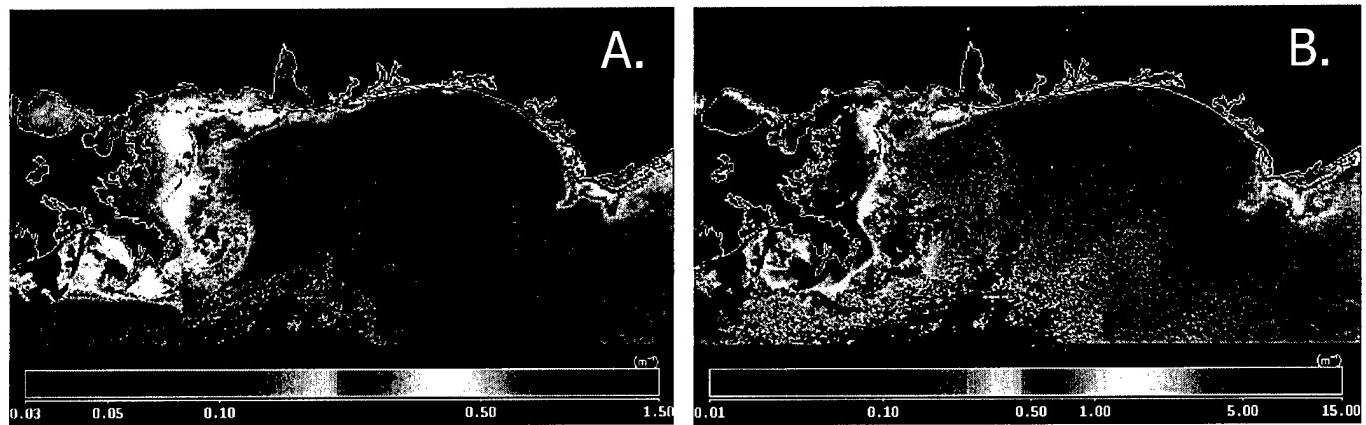
Total scattering at 555 nm can be estimated from SeaWiFS (after conversion from backscattering, following Gould et al., 1999), so $b_i(555)$ can be calculated by difference. Figures 7A and B show examples of $b_o(555)$ and $b_i(555)$ derived from SeaWiFS imagery collected on 20 May, 2002, during our Mobile Bay experiment.

DISCUSSION AND CONCLUSION

The simple empirical algorithms presented here are a first attempt to derive a_{CDOM} , TSS, POM, and PIM products from SeaWiFS ocean color imagery. Comparison



*Figure 6. SeaWiFS imagery, May 20, 2002. A. POM. B. PIM. C. TSS.
Black pixels are clouds.*



*Figure 7. SeaWiFS imagery, May 20, 2002. A. $b_o(555)$. B. $b_i(555)$.
Black pixels are clouds.*

of the satellite-derived values with measured values will enable us to assess the validity of the algorithms. In addition, comparison with, or perhaps a blending with, recently derived analytical algorithms to estimate organic and inorganic components (Twardowski et al., 2001) may also improve the satellite estimates. As the satellite estimates of POM and PIM are based on derived estimates of particulate absorption (which in turn are based on the satellite estimates of total absorption and CDOM absorption), they will only be as good as the original absorption estimates. In the past, we have generally found the satellite absorption values to underestimate the true, measured values, so we can expect the second-order products based on these absorption values to underestimate the true values as well. Nevertheless, interesting patterns are apparent in the imagery. For example, in the offshore waters of Mississippi Bight, POM concentrations exceed PIM concentrations, whereas in coastal waters PIM greatly exceeds POM (Figure 6).

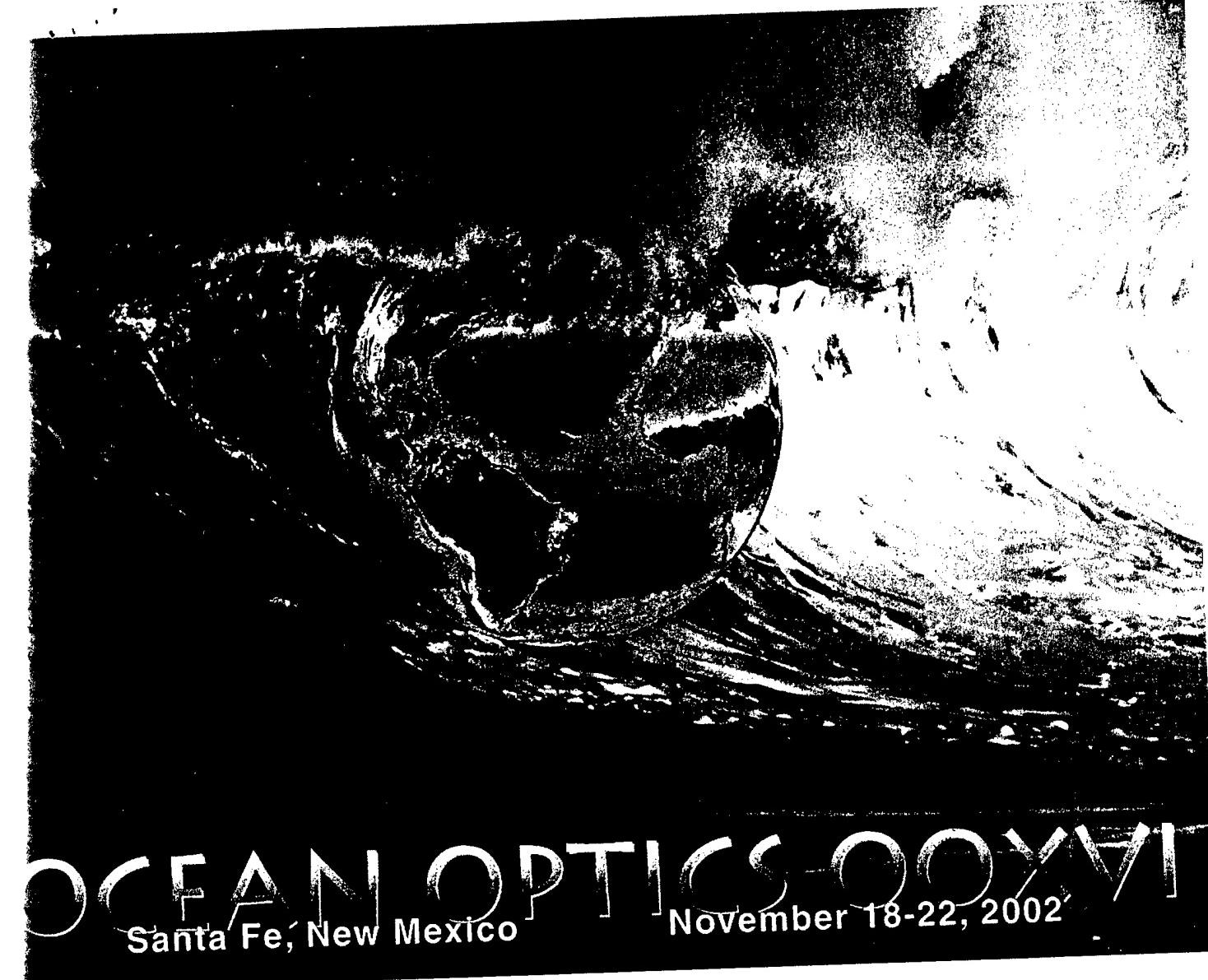
Separating the absorption and scattering coefficients into dissolved and particulate components, and further into organic and inorganic constituents, is an important step toward furthering our understanding of the carbon cycle, particularly in coastal zones.

ACKNOWLEDGMENTS

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